

# A New Method of Calculating the Spin-Wave Velocity $c$ of Spin-1/2 Antiferromagnets With $O(N)$ Symmetry in a Monte Carlo Simulation

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Motivated by the so-called cubical regime in magnon chiral perturbation theory, we propose a new method to calculate the low-energy constant, namely the spin-wave velocity  $c$  of spin-1/2 antiferromagnets with  $O(N)$  symmetry in a Monte Carlo simulation. Specifically we suggest that  $c$  can be determined by  $c = L/\beta$  when the squares of the spatial and temporal winding numbers are tuned to be the same in the Monte Carlo calculations. Here  $\beta$  and  $L$  are the inverse temperature and the box size used in the simulations when this condition is met. We verify the validity of this idea by simulating the quantum spin-1/2 XY model. The  $c$  obtained by using the squares of winding numbers is given by  $c = 1.1348(5)Ja$  which is consistent with the known values of  $c$  in the literature. Unlike other conventional approaches, our new idea provides a direct method to measure  $c$ . Further, by simultaneously fitting our Monte Carlo data of susceptibilities  $\chi_{11}$  and spin susceptibilities  $\chi$  to their theoretical predictions from magnon chiral perturbation theory, we find  $c$  is given by  $c = 1.1347(2)Ja$  which agrees with the one we obtain by the new method of using the squares of winding numbers. The low-energy constants magnetization density  $\mathcal{M}$  and spin stiffness  $\rho$  of quantum spin-1/2 XY model are determined as well and are given by  $\mathcal{M} = 0.43561(1)/a^2$  and  $\rho = 0.26974(5)J$ , respectively. Thanks to the prediction power of magnon chiral perturbation theory which puts a very restricted constraint among the low-energy constants for the model considered here, the accuracy of  $\mathcal{M}$  we present in this study is much precise than previous Monte Carlo result.

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## INTRODUCTION

During the last twenty years, models with  $O(N)$  symmetry which are relevant to antiferromagnets have drawn a lot of attention. In particular spin-1/2 Heisenberg-type models have been studied in great detail both analytically and numerically because it is believed that these models are the correct models to describe the undoped precursors of high  $T_c$  cuprates (undoped antiferromagnets). Beside their phenomenological importance, these  $O(N)$  models for antiferromagnets are interesting from theoretical perspective as well. Further, because of the availability of efficient Monte Carlo algorithms and increasing computing power, the physics of these models has been investigated with unprecedented numerical accuracy [1–10]. For instance, using a loop algorithm as well as finite-volume and -temperature predictions from magnon chiral perturbation theory, the corresponding low-energy constants, namely the staggered magnetization density  $\mathcal{M}_s$ , the spin stiffness  $\rho_s$  and the spin-wave velocity  $c$  of spin-1/2 Heisenberg model on the square lattices are determined with high accuracy and are in agreement with experimental results [11]. Because the properties of these models with  $O(N)$  symmetry are well-studied, they are particular suitable for exploring any new idea.

In analogy to chiral perturbation theory for the pions in QCD, a systematic low-energy effective field theory for the magnons in an antiferromagnet exists as well and is called magnon chiral perturbation theory [12–14]. Low-energy effective field theories are based on symmetry constraints of the underlying models and are universally applicable. Results obtained by effective field theories are

exact, order by order in a systematic low-energy expansion. Material specific properties enter the effective Lagrangian in the form of a priori undetermined low-energy parameters, like the spin stiffness  $\rho$  ( $\rho_s$ ) or the spin-wave velocity  $c$ . Once the numerical values of these low-energy constants are determined, either by Monte Carlo simulations or experimental data, the low-energy physics of the underlying models are completely determined. Since the low-energy physics of the underlying model only depends on the corresponding low-energy constants, it is important to determine these low-energy constants as precise as possible. From theoretical perspective, to determine the numerical values of these low-energy constants are important as well. For instance, by simulating spin-1/2 Heisenberg model with an external staggered field on an exactly cubical space-time box (which requires a very precise value of  $c$ ), in addition to being able to determine the numerical values of  $\mathcal{M}_s$  and  $\rho_s$ , such investigation also provides a good opportunity to exam the validity of predictions from the corresponding low-energy effective field theories [15, 16].

For (sub-lattice) magnetization density and spin stiffness, one can directly measure the related observables and then use experimental finite lattice extrapolation formulae to obtain the bulk values of these 2 low-energy constants. On the other hand, the spin-wave velocity  $c$  is always determined in a less direct manner conventionally. Motivated by the so-called cubical regime (defined later) in magnon chiral perturbation theory [17], we propose a new method to calculate the spin-wave velocity  $c$  of spin-1/2 antiferromagnets with  $O(N)$  symmetry in a

Monte Carlo simulation<sup>1</sup>. Specifically, we propose that  $c$  can be calculated by  $c = L/\beta$  when the squares of spatial and temporal winding numbers are tuned to be the same. Here  $L$  and  $\beta$  are the spatial box size and the inverse temperature used in the simulations when above condition is met. Since this method allows one to measure  $c$  in a direct manner, the result is more accurate than other methods. Indeed as we will demonstrate later, for quantum spin-1/2 XY model, the numerical value of  $c = 1.1348(5)Ja$  we obtain using the new idea is of high precision and is consistent with the known Monte Carlo results in the literature as well [19]. Further, by simultaneously fitting our Monte Carlo data of susceptibilities  $\chi_{11}$  and spin susceptibilities  $\chi$  to their theoretical predictions from magnon chiral perturbation theory [17], we find  $c$  is given by  $c = 1.1347(2)Ja$  which is consistent with the one we obtain by the new method. These results confirm the validity and usefulness of our new method. Additionally other two low-energy constants, namely the magnetization density  $\mathcal{M}$  and spin stiffness  $\rho$  of spin-1/2 XY model are calculated with high accuracy and are much precise than previous Monte Carlo estimates [19].

The remaining of this paper is organized as follows. After a brief introduction to our motivation of this study, we summarize the model and observables investigated here. Follows that we review the corresponding effective field theory predictions relevant to our study. Then we present our numerical results. In particular we demonstrate the validity of the method we used in our simulations to determine the low-energy constant  $c$ . Along the verification, the low-energy constants  $\mathcal{M}$  and  $\rho$  are also calculated. Finally a section is devoted to the conclusion of our investigation.

## MICROSCOPIC MODELS AND CORRESPONDING OBSERVABLES

The quantum XY model we consider in this study is defined by the Hamilton operator

$$H = \sum_{\langle i,j \rangle} J \left[ S_i^1 S_j^1 + S_i^2 S_j^2 \right], \quad (1)$$

where  $S_i^1$  and  $S_i^2$  are the first and second components of a spin-1/2 operator at site  $i$ , and  $i, j$  denotes a pair of nearest neighbor sites on a square lattice. Further,  $J$  in eq. (1) is the antiferromagnetic coupling. A physical quantity of central interest is the susceptibility which is

given by

$$\chi_{11} = \frac{1}{L^2} \int_0^\beta dt \frac{1}{Z} \text{Tr}[M^1(0)M^1(t) \exp(-\beta H)]. \quad (2)$$

Here  $\beta$  is the inverse temperature,  $L$  is the spatial box size,  $Z = \text{Tr} \exp(-\beta H)$  is the partition function and  $M^1 = \sum_x S_x^1$  is the first component of magnetization. Another relevant quantity is the spin susceptibility which is given by

$$\chi = \frac{1}{L^2} \int_0^\beta dt \frac{1}{Z} \text{Tr}[M^3(0)M^3(t) \exp(-\beta H)], \quad (3)$$

here  $M^3 = \sum_x S_x^3$ . Both  $\chi_{11}$  and  $\chi$  can be measured very efficiently with the loop-cluster algorithm using improved estimators [11]. In particular, in the multi-cluster version of the algorithm the susceptibility is given in terms of the cluster sizes  $|\mathcal{C}|$ , i.e.  $\chi_{11} = \frac{1}{\beta L^2} \langle \sum_{\mathcal{C}} |\mathcal{C}|^2 \rangle$ . Similarly, the spin susceptibility  $\chi = \frac{\beta}{L^2} \langle W_t^2 \rangle = \frac{\beta}{L^2} \langle \sum_{\mathcal{C}} W_t(\mathcal{C})^2 \rangle$  is given in terms of the temporal winding number  $W_t = \sum_{\mathcal{C}} W_t(\mathcal{C})$  which is the sum of winding numbers  $W_t(\mathcal{C})$  of the loop-clusters  $\mathcal{C}$  around the Euclidean time direction. Finally, the spatial winding numbers are defined by  $W_i = \sum_{\mathcal{C}} W_i(\mathcal{C})$  with  $i \in \{1, 2\}$ .

## LOW-ENERGY EFFECTIVE THEORY FOR MAGNONS

Due to the spontaneous breaking of the global  $O(2)$  symmetry, the low-energy physics of antiferromagnets with an  $O(2)$  symmetry is governed by one massless Goldstone boson. Detailed calculations of a variety of physical quantities for the spin-1/2 antiferromagnets with  $O(N)$  symmetry including the NNLO contributions have been carried out in [17]. Here we only quote the results that are relevant to our study. The aspect ratio of a spatially quadratic space-time box with box size  $L$  is characterized by  $l = (\beta c/L)^{1/3}$ , with which one distinguishes cubical space-time volumes with  $\beta c \approx L$  from cylindrical ones with  $\beta c \gg L$ . The  $c$  appearing above is the low-energy constant spin-wave velocity. In the cubical regime, the volume- and temperature-dependence of the susceptibility is given by

$$\begin{aligned} \chi_{11} = & \frac{\mathcal{M}^2 L^2 \beta}{2} \left\{ 1 + \frac{c}{\rho_s L l} \beta_1(l) \right. \\ & + \frac{1}{2} \left( \frac{c}{\rho_s L l} \right)^2 [\beta_1(l)^2 \\ & + \beta_2(l)] + O\left(\frac{1}{L^3}\right) \Big\}, \end{aligned} \quad (4)$$

where  $\mathcal{M}$  is the magnetization density and  $\rho$  is the spin stiffness. Further the spin susceptibility in the cubical regime takes the form

$$\chi = \frac{\rho}{c^2} \left\{ 1 + O\left(\frac{1}{L^3}\right) \right\}. \quad (5)$$

<sup>1</sup> This method was implicitly used in [18] for the study of constraint effective potentials. Here we carry out quantitative investigation to verified the validity of this method.

In eq. (4), the functions  $\beta_i(l)$ , which only depend on  $l$ , are shape coefficients of the space-time box defined in [17]. Finally, in the cylindrical regime, the temperature- and volume-dependence of the spin susceptibility  $\chi$  at very low temperature, namely when the condition  $L^2\rho/(\beta c^2) \ll 1$  is satisfied, is given by

$$\chi = 2\frac{\beta}{L^2} \exp\left[-\frac{1}{2}\frac{c^2\beta}{\rho L^2}\right]. \quad (6)$$

## THE DETERMINATION OF THE LOW-ENERGY CONSTANTS

Conventionally the spin-wave velocity  $c$  is determined indirectly in a Monte Carlo simulation. For example, magnon chiral perturbation theory predicts that the finite-volume dependence of the ground state internal energy density is given by [17]

$$e_0(L) = e_0 + 0.7188725c/L^3 + O(1/L^5). \quad (7)$$

By fitting the related Monte Carlo data to above equation,  $c$  can be obtained from the coefficient associated with the term of  $1/L^3$  in eq. (7). Further,  $c$  can be calculated by the standard hydrodynamic relation  $\chi = \rho/c^2$  as well. Notice for both methods mentioned above, extrapolations to infinite volume limit are necessary in order to obtain the numerical value of  $c$ . In other word,  $c$  is determined indirectly and the step of extraoplations will introduce systematic uncertainties into its numerical value. Because of this, here we propose a new method to calculate the numerical value of  $c$  for the spin-1/2 antiferromagnetic models with  $O(N)$  symmetry directly in a Monte Carlo simulation. Our new idea is motivated by the so-called cubical regime in magon chiral perturbation theory [17]. Specifically in magon chiral perturbation theory, an exactly cubical space-time box is obtained through the condition  $\beta c = L$ , here again  $\beta$  and  $L$  are the inverse temperature and the spatial box size, respectively. Further, in a Monte Carlo calculation, if one simulates the system in an exactly cubical space-time box, then the average of the square of spatial winding numbers  $\langle W^2 \rangle = 1/2(\langle W_1^2 \rangle + \langle W_2^2 \rangle)$  and the square of temporal winding number  $\langle W_t^2 \rangle$  should be the same. Once the condition  $\langle W^2 \rangle = \langle W_t^2 \rangle$  is met,  $c$  can be determined by  $c = L/\beta$ . In practice, to employ this new method to calculate  $c$ , for a given box size  $L$ , one varied  $\beta$  until the condition  $\langle W^2 \rangle = \langle W_t^2 \rangle$  is reached. We would like to emphasize that the method we propose here to determine the low-energy constant  $c$  applies to any quantum spin-1/2 antiferromagnetic system with a spontaneous symmetry breaking from a global  $O(N)$  symmetry to its  $O(N-1)$  subgroup. Notice since the  $c$  in the criterion of an exactly cubical space-time box, namely  $\beta c = L$  is its bulk value, one would expect the  $c$  calculated by this new method

suffers very mild finite lattice effects. Indeed, as we will demonstrate shortly, for the quantum XY model considered in this study, th numerical value of  $c$  obtained by the new method is saturated to its bulk value even at  $L = 24a$ .

To verify the validity of the new method we propose here to calculate  $c$  in Monte Carlo simulations, we have carried out several simulations using a continuum-time loop algorithm with  $L = 24a, 32a$  and  $L = 48a$ . Further, by tuning the inverse temperature  $\beta$  for each simulations to reach an exactly cubical space-time box, the numerical values for  $c$  determined from these simulations with  $L = 24a, 32a, 48a$ , are given by  $c = 1.1349(8)Ja$ ,  $c = 1.1347(10)Ja$  and  $c = 1.1347(7)Ja$ , respectively. Figure 1 demonstrates the results of such calculations. The 3 values for  $c$  obtained at different box sizes are consistent with each other and agree with earlier Monte Carlo result of  $c$  as well [19]. This provides a convinving evidence to support the validity of our new method of calculating  $c$  from the squares of spatial and temporal winding numbers. By a weighted average over these values of  $c$  determined at different box sizes, the final result of the numerical value for the low-energy constant  $c$  in this study obtained by the new method is given  $c = 1.1348(5)Ja$ . We have additionally carried out simulations with  $L = 72a$  and  $\beta = 63.450099141/J$  (which corresponds to  $c = 1.13475Ja$ ). The  $\langle W^2 \rangle$  and  $\langle W_t^2 \rangle$  obtained from these new runs are given by 17.1150(95) and 17.109(16), respectively. This result implies that the method of calculating  $c$  through the squares of spatial and temporal winding numbers indeed suffers very mild finite volume effects, at least for the model considered in this study. We notice that the  $\rho$  corresponding to these new runs is given by  $\rho = 0.26973(15)J$  which is statistically consistent with  $\rho = 0.26975(8)J$  calculated at  $L = 24a$ .

Another way to exam whether the new idea of calculating  $c$  through the squares of winding numbers is quantitatively correct is to extract  $c$  by fitting Monte Carlo data of  $\chi_{11}$  and  $\chi$  in the cubical regime to their predicted volume- and temperature-dependence, namely eqs. (4) and (5), respectively. However notice since  $c$  always appears as the quantity  $c/\rho$  or  $\rho^2/c$  in eqs. (4) and (5),  $c$  and  $\rho$  are highly correlated and it would be a challenge to extract  $c$  accurately from the fits. Fortunately we observe from our Monte Carlo data that the observable  $\langle W^2 \rangle$  which is exactly  $\rho\beta$  when  $L \rightarrow \infty$  already reaches a constant for  $L \geq 24a$ . Hence in our simultaneous fits, we also include an improved estimate of the  $\langle W^2 \rangle/\beta$  data obtained earlier when determining  $c$  using the new method and fit these data points to a constant. By simultaneously fitting cubical regime data of  $\chi_{11}$  and  $\chi$  with  $L \geq 24a$  as well as the data of  $\langle W^2 \rangle/\beta$  to their predicted volume- and temperature-dependence formulae, we arrive at  $\mathcal{M} = 0.43561(1)/a^2$ ,  $\rho = 0.26974(5)J$  and  $c = 1.1347(2)Ja$  with a  $\chi^2/\text{d.o.f.} \sim 1$ . The results of

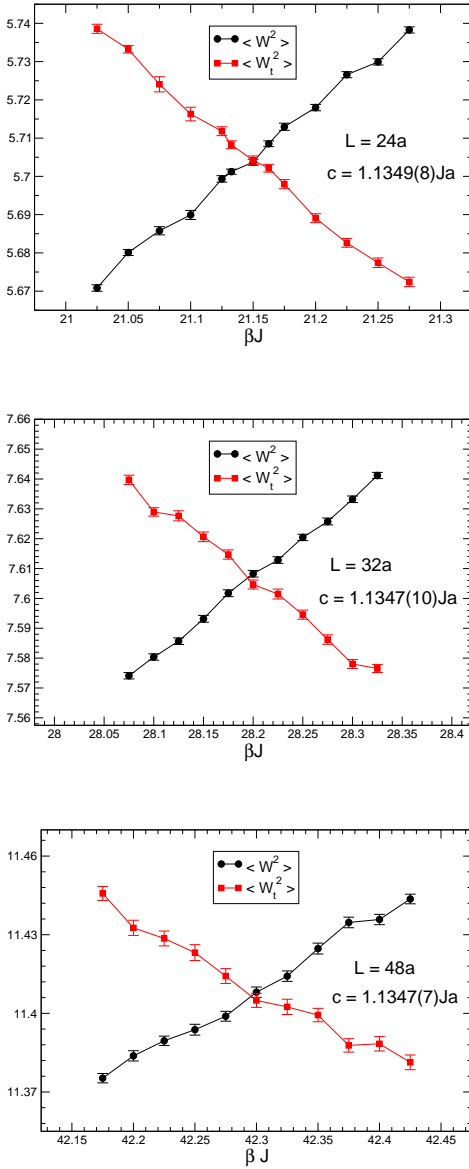


FIG. 1: The determination of  $c$  using the squares of spatial and temporal winding numbers.

the fit are shown in figures 2, 3 and 4. The value of  $c$  calculated from the chiral fits agree nicely with the one determined using the new method. Using large volume data points ( $L \geq 40a$ ) for the fits leads to consistent results. This in turn proves the quantitative correctness of the new method of determining  $c$  using the squares of winding numbers. Notice the values for  $\mathcal{M}$  and  $\rho$  we obtain are consistent with the known values from Monte Carlo simulations [19]. They are in good agreement with the related results from series expansion and spin-wave calculations in the literature as well [20]. Further, the numerical values of these low-energy constants we obtain are much precise than those calculated in earlier Monte Carlo

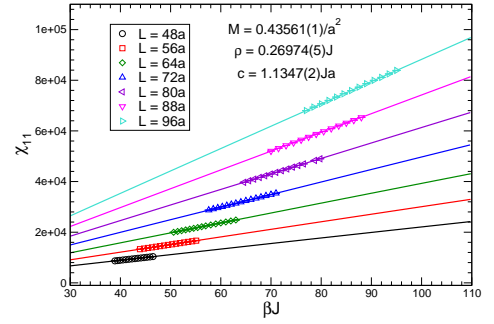


FIG. 2: Result of fitting the data points of  $\chi_{11}$  obtained in the cubical regime to their magnon chiral perturbation theory prediction. Some data points are omitted for better visibility.

study. Finally using the values for  $\rho$  and  $c$  determined in the cubical regime as well as eq. (6), we have compared the theoretical prediction and Monte Carlo data for  $\chi$  in the cylindrical regime. The result of such comparison is shown in figure 5. Considering the fact that there is no free parameter, the agreement demonstrated in figure 5 is reasonably good. All the results presented in this study also provides a strong support for the prediction power and quantitative correctness of magnon chiral perturbation theory in understanding the low-energy physics of the underlying model.

## CONCLUSIONS

In this paper we have proposed a new method to calculate the low-energy constant, namely the spin-wave velocity  $c$  for general antiferromagnetic spin systems with a spontaneous symmetry breaking from a global  $O(N)$  symmetry to its  $O(N-1)$  subgroup using the squares of spatial and temporal winding numbers. We have demonstrated the validity of this method by simulating the quantum spin-1/2 XY model. The numerical value of  $c$  we calculate with the new idea is given by  $c = 1.1348(5)Ja$  which is consistent with the known Monte Carlo result in the literature. By fitting our Monte Carlo data of  $\chi_{11}$  and  $\chi$  to their volume- and temperature-dependence predictions from magnon chiral perturbation theory, we reach  $\mathcal{M} = 0.43561(1)/a^2$ ,  $\rho = 0.26974(5)J$  and  $c = 1.1347(2)Ja$ . The value of  $c$  obtained from the fit is consistent with the one determined by the new method using winding numbers squared. This supports strongly the quantitative correctness of the new method we propose here to calculate the low-energy constant spin-wave velocity  $c$  in Monte Carlo simulations. The idea of using winding number squared is simple, but very powerful and requires moderate computational effort to obtain a very precise numerical value for  $c$ . Finally thanks to the robustness nature and prediction power of magnon chiral perturbation theory which

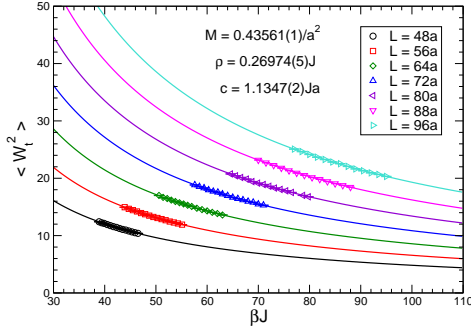


FIG. 3: Result of fitting the data points of  $\langle W_t^2 \rangle$  obtained in the cubical regime to their magnon chiral perturbation theory prediction. Some data points are omitted for better visibility.

puts very restricted constraints on the low-energy constants and observables considered here, we are able to fit simultaneously our finite temperature data points to their predicted formulae from magnon chiral perturbation theory and obtain very accurate values for  $\mathcal{M}$ ,  $\rho$  and  $c$ . The agreement between theoretical prediction and Monte Carlo results of  $\chi$  at very low temperature shown in figure 5 is remarkable as well considering the fact that there is no free parameter in obtaining figure 5.

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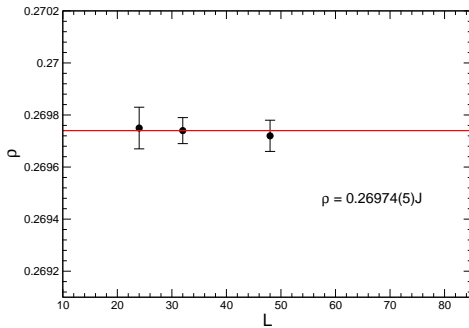


FIG. 4: Result of fitting the data points of  $\rho$  obtained in the cubical regime to a constant.

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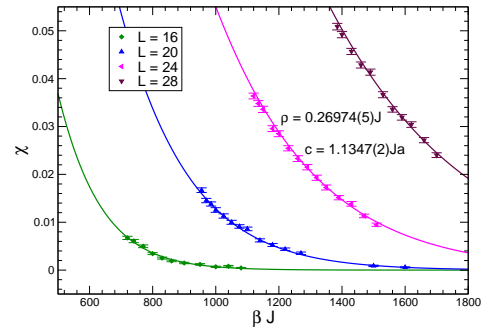


FIG. 5: Comparison between theoretical prediction and Monte Carlo data for  $\chi$  in the cylindrical regime.

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